

TABLE A-3-101

## CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE DIBROMIDE (106-93-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	187.88
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	282.1
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b).	--	1.00E-02 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	4.20E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.47E-04
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.17E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.19E-05
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	5.62E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	3.28E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.28E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.46E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.31E+00

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## CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE DIBROMIDE (106-93-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.15E+01
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	3.50E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.77E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.77E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	9.13E-03
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	9.13E-03

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## CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE DIBROMIDE (106-93-4)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	4.47E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.41E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.71E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	4.47E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.12E-06
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.26E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1996c)	C-1-8	5.70E-05
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	8.50E+01
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1995b)	C-2-3	2.00E-04
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S. EPA (1997b)	C-2-1	2.20E-04
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	Calculated from $Inhalation URF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-2	7.70E-01

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-102

## CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE OXIDE (75-21-8)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	44.05
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	162.1
$V_p$ (atm)	Verschueren (1983)	--	1.44E+00 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in NC DEHNR (1996).	--	3.80E+05
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.67E-04
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.71E-01
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.44E-05
$K_{ow}$ (unitless)	Howard (1989-1993)	--	5.01E-01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	8.26E-01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.26E-03
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.19E-02
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.30E-02

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## CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE OXIDE (75-21-8)

Parameter	Reference and Explanation	Equations	Value
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	2.13E+01
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.44E+00
$Br_{root \text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	7.80E+02
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	5.77E+01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	5.77E+01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.60E-04
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.60E-04

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## CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE OXIDE (75-21-8)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	3.98E-09
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.26E-08
<b>Biotransfer Factors for Animals (Continued)</b>			
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	1.52E-08
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	3.98E-06
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	9.94E-09
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	3.48E-01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-1-7	1.02E+00
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S. EPA (1997c)	C-2-1	1.0E-04
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	3.5E-01

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-103

## CHEMICAL-SPECIFIC INPUTS FOR BIS(2-ETHYLHEXYL)PHTHALATE (117-81-7)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	390.54
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	218.1
$V_p$ (atm)	$V_p$ value cited in Montgomery and Welkom (1991).	--	1.12E-11 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1992a).	--	3.96E-01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.10E-08
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.32E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	4.22E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.60E+05
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.11E+09
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.11E+03
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.33E+03
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	4.44E+03

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## CHEMICAL-SPECIFIC INPUTS FOR BIS(2-ETHYLHEXYL)PHTHALATE (117-81-7)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.10E+01
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.37E+03
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	2.13E+00
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.80E-02
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.80E-02
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.77E+06
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.77E+06



TABLE A-3-103

## CHEMICAL-SPECIFIC INPUTS FOR BIS(2-ETHYLHEXYL)PHTHALATE (117-81-7)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.27E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	4.03E-03
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	4.88E-03
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.27E+00
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	3.18E-03
$BCF_{fish}$ (L/kg, FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	3.60E+02
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.00E-02
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S.EPA (1997b)	C-1-7	1.40E-02
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	7.00E-02
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	4.00E-06
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	1.4E-02

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-104

## CHEMICAL-SPECIFIC INPUTS FOR FLUORANTHENE (206-44-0)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	202.26
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	383.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.07E-08 at 25°C (solid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	2.32E-01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	9.33E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.75E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.18E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	1.21E+05
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	4.91E+04
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.91E+02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.68E+03
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.96E+03

TABLE A-3-104

## CHEMICAL-SPECIFIC INPUTS FOR FLUORANTHENE (206-44-0)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	5.75E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.992
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.92E+03
$Br_{root \text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	3.90E+00
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	4.46E-02
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	4.46E-02
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.56E+03
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.56E+03

TABLE A-3-104

## CHEMICAL-SPECIFIC INPUTS FOR FLUORANTHENE (206-44-0)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	9.65E-04
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.05E-03
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	3.69E-03
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	9.65E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.41E-03
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Carroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	1.57E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	4.0E-02
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.4E-01
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-105

## CHEMICAL-SPECIFIC INPUTS FOR FLUORENE (86-73-7)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	166.22
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	389.1
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1992a).	--	1.08E-09 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1992a).	--	1.90E+00
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	9.41E-08
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.63E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-4-20	7.88E-06
$K_{ow}$ (unitless)	$K_{ow}$ value cited in U.S. EPA (1995b)	--	1.47E+04
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	7.71E+03
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.71E+01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.78E+02
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.08E+02

TABLE A-3-105

## CHEMICAL-SPECIFIC INPUTS FOR FLUORENE (86-73-7)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	4.22E+00
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.935
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.83E+02
$Br_{root \text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $K_{ds}$ value provided in this table.	B-2-10	4.96E+00
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.51E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.51E-01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.63E+04
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.63E+04

TABLE A-3-105

## CHEMICAL-SPECIFIC INPUTS FOR FLUORENE (86-73-7)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.17E-04
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.70E-04
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	4.48E-04
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.17E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.92E-04
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Carroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	1.20E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1997b)	C-1-8	4.00E-02
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.40E-01
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-106

## CHEMICAL-SPECIFIC INPUTS FOR FORMALDEHYDE (50-00-0)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	30.03
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	365.1
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1994c)	--	5.10E+00 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b)	--	5.50E+05
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.78E-04
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.00E-01
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-4-20	1.74E-05
$K_{ow}$ (unitless)	$K_{ow}$ value cited in U.S. EPA (1995b)	--	2.20E+00
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	2.62E+00
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.62E-02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.96E-01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.05E-01



TABLE A-3-106

## CHEMICAL-SPECIFIC INPUTS FOR FORMALDEHYDE (50-00-0)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.73E+00
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	2.57E+02
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.46E+01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for above ground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.46E+01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	4.65E-04
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	4.65E-04

TABLE A-3-106

## CHEMICAL-SPECIFIC INPUTS FOR FORMALDEHYDE (50-00-0)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.75E-08
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	5.53E-08
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	6.69E-08
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.75E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	4.36E-08
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF$ values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—See Appendix A-3.	B-4-26	1.07E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.00E-01
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	Calculated from $Inhalation\ URF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-1-7	4.50E-02
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	7.00E-01
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S.EPA (1997b)	C-2-1	1.30E-05
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S.EPA (1997c)	C-2-2	4.50E-02

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-107

## CHEMICAL-SPECIFIC INPUTS FOR FORMIC ACID (64-18-6)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	U.S. EPA (1995b)	--	46.03
$T_m$ (K)	U.S. EPA (1995b)	--	282.0
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b)	--	5.40E-02 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b)	--	1.00E+06
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.49E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.22E-01
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.71E-05
$K_{ow}$ (unitless)	$K_{ow}$ value cited in U.S. EPA (1995b)	--	2.90E-01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	5.39E+00
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.39E-02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	4.04E-01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.16E-01

TABLE A-3-107

## CHEMICAL-SPECIFIC INPUTS FOR FORMIC ACID (64-18-6)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	3.61E+01
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	6.40E+00
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	1.19E+02
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	7.92E+01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	7.92E+01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	6.02E-03
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	6.02E-03

TABLE A-3-107

## CHEMICAL-SPECIFIC INPUTS FOR FORMIC ACID (64-18-6)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.30E-09
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	7.28E-09
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	8.82E-09
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.30E-06
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	5.75E-09
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	2.30E-01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997c)	C-1-8	2.00E+00
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	7.00E+00
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-108

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,6,7,8-HEPTACHLORODIBENZO(P)DIOXIN (35822-46-9)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	U.S. EPA (1994a)	--	425.31
$T_m$ (K)	U.S. EPA (1994a)	--	537.1
$Vp$ (atm)	U.S. EPA (1994a)	--	4.22E-14 at 25°C (solid)
$S$ (mg/L)	U.S. EPA (1994a)	--	2.40E-06
$H$ (atm·m <sup>3</sup> /mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.50E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.11E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	3.89E-06
$K_{ow}$ (unitless)	U.S. EPA (1992d)	--	1.58E+08
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	9.77E+07
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.77E+05
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.33E+06

TABLE A-3-108

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,6,7,8-HEPTACHLORODIBENZO(P)DIOXIN (35822-46-9)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.91E+06
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.09E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.62E-02
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	4.79E+05
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	4.90E-01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	7.05E-04
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	7.05E-04
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	3.50E+05

TABLE A-3-108

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,6,7,8-HEPTACHLORODIBENZO(P)DIOXIN (35822-46-9)**

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (Continued)</b>			
$Bv_{forage}$ $\left(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ air}}\right)$	$Bv_{forage}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	3.50E+05
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	U.S. EPA (1995a)	B-3-11	1.00E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	5.4E-03
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	6.57E-03
$Ba_{egg}$ (L/kg FW tissue)	$Ba_{egg}$ value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	2.55E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	8.58E-03
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	5.00E-03
<b>Other Parameters</b>			
$TEF$ (unitless)	U.S. EPA (1994a)	--	0.01
<b>Health Benchmarks</b>			
$Oral \text{ CSF}$ (mg/kg/day) <sup>-1</sup>	--	C-1-8	ND
$Inhalation \text{ CSF}$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfD$ (mg/kg/day)	--	C-2-3	ND
$Inhalation \text{ URF}$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$RfC$ (mg/m <sup>3</sup> )	--	C-2-2	ND



**TABLE A-3-108**

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,6,7,8-HEPTACHLORODIBENZO(P)DIOXIN (35822-46-9)**

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Note:

NA = Not Applicable; ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-109

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,6,7,8-HEPTACHLORODIBENZO(P)FURAN (67562-39-4)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	U.S. EPA (1994a)	--	409.31
$T_m$ (K)	U.S. EPA (1994a)	--	509.1
$V_p$ (atm)	U.S. EPA (1994a)	--	1.75E-13 at 25°C (solid)
$S$ (mg/L)	U.S. EPA (1994a)	--	1.35E-06
$H$ (atm·m <sup>3</sup> /mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.30E-05
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated by using Equation A-3-2. Recommended value was calculated by using the $MW$ and $D_a$ values that are provided in the tables in Appendix A-3 for 2,3,7,8-TCDF.	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.55E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	3.99E-06
$K_{ow}$ (unitless)	U.S. EPA (1992d)	--	8.32E+07
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	5.13E+07
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.13E+05
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.85E+06

TABLE A-3-109

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,6,7,8-HEPTACHLORODIBENZO(P)FURAN (67562-39-4)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.05E+06
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	3.57E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	3.47E-02
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.91E+05
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	5.68E-01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.02E-03
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.02E-03
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	4.40E+05

TABLE A-3-109

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,6,7,8-HEPTACHLORODIBENZO(P)FURAN (67562-39-4)**

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (Continued)</b>			
$Bv_{forage}$ $\left(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ air}}\right)$	$Bv_{forage}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	4.40E+05
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	U.S. EPA (1995a)	B-3-11	1.00E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	5.43E-03
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	6.57E-03
$Ba_{egg}$ (L/kg FW tissue)	$Ba_{egg}$ value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	2.09E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	7.04E-03
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	5.00E-03
<b>Other Parameters</b>			
$TEF$ (unitless)	U.S. EPA (1994a)	--	0.01
<b>Health Benchmarks</b>			
$Oral \text{ CSF}$ (mg/kg/day) <sup>-1</sup>	--	C-1-8	ND
$Inhalation \text{ CSF}$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfD$ (mg/kg/day)	--	C-2-3	ND
$Inhalation \text{ URF}$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$RfC$ (mg/m <sup>3</sup> )	--	C-2-2	ND

**TABLE A-3-109**

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,6,7,8-HEPTACHLORODIBENZO(P)FURAN (67562-39-4)**

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Note:

NA = Not Applicable; ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-110

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,7,8,9-HEPTACHLORODIBENZO(P)FURAN (55673-89-7)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	U.S. EPA (1994a)	--	409.31
$T_m$ (K)	U.S. EPA (1994a)	--	494.1
$V_p$ (atm)	U.S. EPA (1994a)	--	1.41E-13 at 25°C (solid)
$S$ (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	--	1.40E-06
$H$ (atm·m <sup>3</sup> /mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.30E-05
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated by using Equation A-3-2. Recommended value was calculated by using the $MW$ and $D_a$ values that are provided in the tables in Appendix A-3 for 2,3,7,8-TCDF.	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.55E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	3.99E-06
$K_{ow}$ (unitless)	Homologue group average value obtained from U.S. EPA (1992d).	--	8.32E+07
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	5.13E+07
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.13E+05
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.85E+06

TABLE A-3-110

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,7,8,9-HEPTACHLORODIBENZO(P)FURAN (55673-89-7)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.05E+06
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	3.57E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	2.01E-02
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.91E+05
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	5.68E-01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.02E-03
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.02E-03
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	4.40E+05

TABLE A-3-110

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,7,8,9-HEPTACHLORODIBENZO(P)FURAN (55673-89-7)**

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (Continued)</b>			
$Bv_{forage}$ $\left(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}}\right)$	$Bv_{forage}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	4.40E+05
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	U.S. EPA (1995a)	B-3-11	3.00E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	1.63E-02
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	1.97E-02
$Ba_{egg}$ (L/kg FW tissue)	$Ba_{egg}$ value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	2.42E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	1.06E-02
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	5.00E-03
<b>Other Parameters</b>			
$TEF$ (unitless)	U.S. EPA (1994a)	--	0.01
<b>Health Benchmarks</b>			
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-8	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfD$ (mg/kg/day)	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$RfC$ (mg/m <sup>3</sup> )	--	C-2-2	ND



**TABLE A-3-110**

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,7,8,9-HEPTACHLORODIBENZO(P)FURAN (55673-89-7)**

Note:

NA = Not Applicable; ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-111

## CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR (76-44-8)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	373.35
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	368.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	4.29E-07 at 25°C (solid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	2.73E+01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.87E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.12E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.69E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.04E+05
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	9.53E+03
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.53E+01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.15E+02
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.81E+02

TABLE A-3-111

## CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR (76-44-8)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	1.70E+03
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	1.78E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	4.89E-02
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	4.89E-02
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	2.09E+03
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	2.09E+03

TABLE A-3-111

## CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR (76-44-8)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	8.22E-04
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.60E-03
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	3.15E-03
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	8.22E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	2.05E-03
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF$ values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—See Appendix A-3.	B-4-26	5.52E+03
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.00E-04
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	4.50E+00
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.80E-03
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S. EPA (1997b)	C-2-1	1.30E-03
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	4.50E+00

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-112

## CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR EPOXIDE (1024-57-3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
$MW$ (g/mole)	Montgomery and Welkom (1991)	--	389.32
$T_m$ (K)	Montgomery and Welkom (1991)	--	430.1
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1992a).	--	7.51E-12 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1992a) .	--	2.68E-01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.09E-08
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.32E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	4.23E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	5.62E+04
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	7.18E+03
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.18E+01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.38E+02
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.87E+02

TABLE A-3-112

## CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR EPOXIDE (1024-57-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	4.58E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	2.03E-01
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.06E+03
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	1.48E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	6.96E-02
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	6.96E-02
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	5.86E+05
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	5.86E+05

TABLE A-3-112

## CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR EPOXIDE (1024-57-3)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	4.47E-04
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.41E-03
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.71E-03
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	4.47E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.12E-03
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Carroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	5.88E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1997b)	C-1-8	1.30E-05
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S.EPA (1997b)	C-1-7	9.1E+00
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	4.6E-05
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S.EPA (1997b)	C-2-1	2.6E-03
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	9.1E+00

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-113

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,7,8-HEXACHLORODIBENZO(P)DIOXIN (39227-28-6)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	U.S. EPA (1994a)	--	390.87
$T_m$ (K)	U.S. EPA (1994a)	--	546.1
$Vp$ (atm)	U.S. EPA (1994a)	--	1.33E-13 at 25°C (solid)
$S$ (mg/L)	U.S. EPA (1994a)	--	4.40E-06
$H$ (atm·m <sup>3</sup> /mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.20E-05
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.15E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.12E-06
$K_{ow}$ (unitless)	U.S. EPA (1992d)	--	6.17E+07
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for dioxins and furans that is cited in U.S. EPA (1994a; 1994c). Recommended value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	3.80E+07
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.80E+05
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.85E+06



TABLE A-3-113

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,7,8-HEXACHLORODIBENZO(P)DIOXIN (39227-28-6)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.52E+06
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.09E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	5.96E-02
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.31E+05
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	6.09E-01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.22E-03
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.22E-03
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	4.50E+05

TABLE A-3-113

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,7,8-HEXACHLORODIBENZO(P)DIOXIN (39227-28-6)**

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (Continued)</b>			
$Bv_{forage}$ $\left(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ air}}\right)$	$Bv_{forage}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	4.50E+05
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	U.S. EPA (1995a)	B-3-11	6.00E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	3.26E-02
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	3.94E-02
$Ba_{egg}$ (L/kg FW tissue)	$Ba_{egg}$ value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	4.53E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	4.03E-02
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	4.00E-02
<b>Other Parameters</b>			
$TEF$ (unitless)	U.S. EPA (1994a)	--	0.10
<b>Health Benchmarks</b>			
$Oral \text{ CSF}$ (mg/kg/day) <sup>-1</sup>	--	C-1-8	ND
$Inhalation \text{ CSF}$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfD$ (mg/kg/day)	--	C-2-3	ND
$Inhalation \text{ URF}$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$RfC$ (mg/m <sup>3</sup> )	--	C-2-2	ND

Note:

**TABLE A-3-113**

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,7,8-HEXACHLORODIBENZO(P)DIOXIN (39227-28-6)**

NA = Not Applicable; ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-114

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,6,7,8-HEXACHLORODIBENZO(P)DIOXIN (57653-85-7)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	U.S. EPA (1994a)	--	390.87
$T_m$ (K)	U.S. EPA (1994a)	--	558.1
$Vp$ (atm)	U.S. EPA (1994a)	--	4.74E-14 at 25°C (solid)
$S$ (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	--	4.40E-06
$H$ (atm·m <sup>3</sup> /mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.20E-05
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated by using Equation A-3-2. Recommended value was calculated by using the $MW$ and $D_a$ values that are provided in the tables in Appendix A-3 for 2,3,7,8-TCDD.	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.15E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.12E-06
$K_{ow}$ (unitless)	Homologue group average value obtained from U.S. EPA (1992d).	--	1.78E+07
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.10E+07
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.10E+05
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.22E+05

TABLE A-3-114

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,6,7,8-HEXACHLORODIBENZO(P)DIOXIN (57653-85-7)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	4.39E+05
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value assumed to be the same as the $k_{sg}$ value calculated for 1,2,3,4,7,8-HexaCDD. $k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.09E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	2.89E-02
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.88E+04
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	8.10E-01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.50E-03
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.50E-03
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	4.50E+05

TABLE A-3-114

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,6,7,8-HEXACHLORODIBENZO(P)DIOXIN (57653-85-7)**

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (Continued)</b>			
$Bv_{forage}$ $\left(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}}\right)$	$Bv_{forage}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	4.50E+05
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	U.S. EPA (1995a)	B-3-11	5.00E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	2.71E-02
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	3.29E-02
$Ba_{egg}$ (L/kg FW tissue)	$Ba_{egg}$ value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	3.70E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	2.57E-02
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	4.00E-02
<b>Other Parameters</b>			
$TEF$ (unitless)	U.S. EPA (1994a)	--	0.10
<b>Health Benchmarks</b>			
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-8	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfD$ (mg/kg/day)	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$RfC$ (mg/m <sup>3</sup> )	--	C-2-2	ND

**TABLE A-3-114**

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,6,7,8-HEXACHLORODIBENZO(P)DIOXIN (57653-85-7)**

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Note:

NA = Not Applicable; ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-115

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,7,8,9-HEXACHLORODIBENZO(P)DIOXIN (19408-74-3)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	U.S. EPA (1994a)	--	390.87
$T_m$ (K)	U.S. EPA (1994a)	--	516.1
$Vp$ (atm)	U.S. EPA (1994a)	--	6.45E-14 at 25°C (solid)
$S$ (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	--	4.40E-06
$H$ (atm·m <sup>3</sup> /mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.20E-05
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.15E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.12E-06
$K_{ow}$ (unitless)	Homologue group average value obtained from U.S. EPA (1994a).	--	1.78E+07
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for dioxins and furans that is cited in U.S. EPA (1994a; 1994c). Recommended value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.10E+07
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.10E+05
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.22E+05



TABLE A-3-115

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,7,8,9-HEXACHLORODIBENZO(P)DIOXIN (19408-74-3)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	4.39E+05
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was assumed to be the same as the $k_{sg}$ value for 1,2,3,4,7,8-HexaCDD. $k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.09E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.53E-02
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.88E+04
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	8.10E-01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.50E-03
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.50E-03
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	4.50E+05

TABLE A-3-115

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,7,8,9-HEXACHLORODIBENZO(P)DIOXIN (19408-74-3)**

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants</b>			
$Bv_{forage}$ $\left(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ air}}\right)$	$Bv_{forage}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	4.50E+05
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	U.S. EPA (1995a)	B-3-11	5.00E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	2.71E-02
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	3.29E-02
$Ba_{egg}$ (L/kg FW tissue)	$Ba_{egg}$ value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	2.33E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	1.39E-02
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	4.00E-02
<b>Other Parameters</b>			
$TEF$ (unitless)	U.S. EPA (1994a)	--	0.10
<b>Health Benchmarks</b>			
$Oral \text{ CSF}$ (mg/kg/day) <sup>-1</sup>	--	C-1-8	ND
$Inhalation \text{ CSF}$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfD$ (mg/kg/day)	--	C-2-3	ND
$Inhalation \text{ URF}$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$RfC$ (mg/m <sup>3</sup> )	--	C-2-2	ND

**TABLE A-3-115**

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,7,8,9-HEXACHLORODIBENZO(P)DIOXIN (19408-74-3)**

Note:

NA = Not Applicable; ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-116

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,7,8-HEXACHLORODIBENZO(P)FURAN (70648-26-9)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	U.S. EPA (1994a)	--	374.87
$T_m$ (K)	U.S. EPA (1994a)	--	498.6
$V_p$ (atm)	U.S. EPA (1994a)	--	3.16E-13 at 25°C (solid)
$S$ (mg/L)	U.S. EPA (1994a)	--	8.25E-06
$H$ (atm·m <sup>3</sup> /mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.40E-05
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated by using Equation A-3-2. Recommended value was calculated by using the $MW$ and $D_a$ values that are provided in the tables in Appendix A-3 for 2,3,7,8-TCDF.	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.62E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.23E-06
$K_{ow}$ (unitless)	Homologue group average value obtained from U.S. EPA (1992d)	--	1.78E+07
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.10E+07
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.10E+05
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.22E+05

TABLE A-3-116

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,7,8-HEXACHLORODIBENZO(P)FURAN (70648-26-9)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	4.39E+05
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	4.86E-02
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.88E+04
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	8.10E-01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.50E-03
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.50E-03
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	1.50E+05

TABLE A-3-116

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,7,8-HEXACHLORODIBENZO(P)FURAN (70648-26-9)**

Parameter	Reference and Explanation	Equations	Value
$Bv_{forage}$ $\left(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}}\right)$	$Bv_{forage}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	1.50E+05
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	U.S. EPA (1995a)	B-3-11	7.00E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	3.80E-02
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	4.60E-02
$Ba_{egg}$ (L/kg FW tissue)	$Ba_{egg}$ value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	4.51E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	3.48E-02
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	4.00E-02
<b>Other Parameters</b>			
$TEF$ (unitless)	U.S. EPA (1994a)	--	0.10
<b>Health Benchmarks</b>			
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-8	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfD$ (mg/kg/day)	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$RfC$ (mg/m <sup>3</sup> )	--	C-2-2	ND

**TABLE A-3-116**

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,7,8-HEXACHLORODIBENZO(P)FURAN (70648-26-9)**

Note:

NA = Not Applicable; ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-117

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,6,7,8-HEXACHLORODIBENZO(P)FURAN (57117-44-9)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	U.S. EPA (1994a)	--	374.87
$T_m$ (K)	U.S. EPA (1994a)	--	505.1
$V_p$ (atm)	U.S. EPA (1994a)	--	2.89E-13 at 25°C (solid)
$S$ (mg/L)	U.S. EPA (1994a)	--	1.77E-05
$H$ (atm·m <sup>3</sup> /mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.10E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated by using Equation A-3-2. Recommended value was calculated by using the $MW$ and $D_a$ values that are provided in the tables in Appendix A-3 for 2,3,7,8-TCDF.	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.62E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.23E-06
$K_{ow}$ (unitless)	Homologue groupaverage value obtained from U.S. EPA (1992d)	--	1.78E+07
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.10E+07
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.10E+05
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.22E+05



TABLE A-3-117

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,6,7,8-HEXACHLORODIBENZO(P)FURAN (57117-44-9)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	4.39E+05
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was assumed to be 0 due to a lack of data.	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	0.0
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	5.15E-02
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.88E+04
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	8.10E-01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.50E-03
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.50E-03
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	1.50E+05

TABLE A-3-117

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,6,7,8-HEXACHLORODIBENZO(P)FURAN (57117-44-9)**

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (Continued)</b>			
$Bv_{forage}$ $\left(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}}\right)$	$Bv_{forage}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	1.50E+05
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	U.S. EPA (1995a)	B-3-11	6.00E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	3.26E-02
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	3.94E-02
$Ba_{egg}$ (L/kg FW tissue)	$Ba_{egg}$ value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	4.53E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	3.56E-02
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	4.00E-02
<b>Other Parameters</b>			
$TEF$ (unitless)	U.S. EPA (1994a)	--	0.10
<b>Health Benchmarks</b>			
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-8	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfD$ (mg/kg/day)	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$RfC$ (mg/m <sup>3</sup> )	--	C-2-2	ND

Note:

**TABLE A-3-117**

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,6,7,8-HEXACHLORODIBENZO(P)FURAN (57117-44-9)**

NA = Not Applicable; ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-118

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,7,8,9-HEXACHLORODIBENZO(P)FURAN (72918-21-9)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	U.S. EPA (1994a)	--	374.87
$T_m$ (K)	U.S. EPA (1994a)	--	519.1
$V_p$ (atm)	U.S. EPA (1994a)	--	2.37E-13 at 25°C (solid)
$S$ (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	--	1.30E-05
$H$ (atm·m <sup>3</sup> /mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.00E-05
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated by using Equation A-3-2. Recommended value was calculated by using the $MW$ and $D_a$ values that are provided in the tables in Appendix A-3 for 2,3,7,8-TCDF.	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.62E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.23E-06
$K_{ow}$ (unitless)	Homologue group average value obtained from U.S. EPA (1992d).	--	1.78E+07
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.10E+07
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.10E+05
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.22E+05

TABLE A-3-118

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,7,8,9-HEXACHLORODIBENZO(P)FURAN (72918-21-9)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	4.39E+05
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	5.76E-0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/mL \text{ soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.88E+04
$Br_{rootveg}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	8.10E-01
$Br_{ag}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.50E-03
$Br_{forage}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.50E-03
$Bv_{ag}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ air}})$	$Bv_{ag}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	1.50E+05

TABLE A-3-118

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,7,8,9-HEXACHLORODIBENZO(P)FURAN (72918-21-9)**

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (Continued)</b>			
$Bv_{forage}$ $\left(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}}\right)$	$Bv_{forage}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	1.50E+05
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	U.S. EPA (1995a)	B-3-11	6.00E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	3.26E-02
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	3.94E-02
$Ba_{egg}$ (L/kg FW tissue)	$Ba_{egg}$ value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	ND
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	ND
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	4.00E-02
<b>Other Parameters</b>			
$TEF$ (unitless)	U.S. EPA (1994a)	--	0.10
<b>Health Benchmarks</b>			
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-8	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfD$ (mg/kg/day)	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$RfC$ (mg/m <sup>3</sup> )	--	C-2-2	ND

TABLE A-3-119

**CHEMICAL-SPECIFIC INPUTS FOR  
2,3,4,6,7,8-HEXACHLORODIBENZO(P)FURAN (60851-34-5)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	U.S. EPA (1994a)	--	374.87
$T_m$ (K)	U.S. EPA (1994a)	--	512.1
$V_p$ (atm)	U.S. EPA (1994a)	--	2.63E-13 at 25°C (solid)
$S$ (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	--	1.30E-05
$H$ (atm·m <sup>3</sup> /mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.00E-05
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated by using Equation A-3-2. Recommended value was calculated by using the $MW$ and $D_a$ values that are provided in the tables in Appendix A-3 for 2,3,7,8-TCDF.	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.62E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.23E-06
$K_{ow}$ (unitless)	Homologue group average value obtained from U.S. EPA (1992d).	--	1.78E+07
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.10E+07
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.10E+05
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.22E+05

TABLE A-3-119

**CHEMICAL-SPECIFIC INPUTS FOR  
2,3,4,6,7,8-HEXACHLORODIBENZO(P)FURAN (60851-34-5)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	4.39E+05
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was assumed to be 0 due to a lack of data.	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	0.0
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	5.47E-02
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.88E+04
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	8.10E-01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.50E-03
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.50E-03
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	1.50E+05



TABLE A-3-119

**CHEMICAL-SPECIFIC INPUTS FOR  
2,3,4,6,7,8-HEXACHLORODIBENZO(P)FURAN (60851-34-5)**

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (Continued)</b>			
$Bv_{forage}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ air}})$	$Bv_{forage}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	1.50E+05
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	U.S. EPA (1995a)	B-3-11	5.00E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	2.71E-02
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	3.29E-02
$Ba_{egg}$ (L/kg FW tissue)	$Ba_{egg}$ value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	2.11E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	1.74E-02
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	4.00E-02
<b>Other Parameters</b>			
$TEF$ (unitless)	U.S. EPA (1994a)	--	0.10
<b>Health Benchmarks</b>			
$Oral \text{ CSF}$ (mg/kg/day) <sup>-1</sup>	--	C-1-8	ND
$Inhalation \text{ CSF}$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfD$ (mg/kg/day)	--	C-2-3	ND
$Inhalation \text{ URF}$ ( $\mu\text{g}/\text{m}^3$ ) <sup>-1</sup>	--	C-2-1	ND
$RfC$ (mg/m <sup>3</sup> )	--	C-2-2	ND

**TABLE A-3-119**

**CHEMICAL-SPECIFIC INPUTS FOR  
2,3,4,6,7,8-HEXACHLORODIBENZO(P)FURAN (60851-34-5)**

Note:

NA = Not Applicable; ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-120

**CHEMICAL-SPECIFIC INPUTS FOR HEXACHLORO-1,3-BUTADIENE  
(PERCHLOROBUTADIENE) (87-68-3)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Montgomery and Welkom (1991)	--	260.76
$T_m$ (K)	Montgomery and Welkom (1991)	--	252.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.33E-04 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	2.54E+00
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.39E-02
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.73E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.33E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	5.38E+04
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	6.94E+03
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	6.94E+01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.20E+02
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.77E+02

TABLE A-3-120

**CHEMICAL-SPECIFIC INPUTS FOR HEXACHLORO-1,3-BUTADIENE  
(PERCHLOROBUTADIENE) (87-68-3)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.03E+03
$Br_{root \text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	1.48E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	7.14E-02
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	7.14E-02
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	2.55E-01
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	2.55E-01

TABLE A-3-120

**CHEMICAL-SPECIFIC INPUTS FOR HEXACHLORO-1,3-BUTADIENE  
(PERCHLOROBUTADIENE) (87-68-3)**

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	4.28E-04
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.35E-03
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.64E-03
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	4.27E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.07E-03
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Carroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	5.69E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1995b)	C-1-8	2.00E-04
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	7.80E-02
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	7.00E-04
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S. EPA (1997b)	C-2-1	2.20E-05
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	7.80E-02

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-121

## CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROBENZENE (118-74-1)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	284.8
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	504.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	1.62E-08 at 25°C (solid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	8.62E-03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.35E-04
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.41E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-4-20	7.84E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	3.18E+05
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	8.00E+04
$Kd_s$ (mL/g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.00E+02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.00E+03
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.20E+03

TABLE A-3-121

## CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROBENZENE (118-74-1)

Parameter	Reference and Explanation	Equations	Value
<b>Cemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.21E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	4.02E+03
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	5.02E+00
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.56E-02
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.56E-02
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	7.57E+01
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	7.57E+01

TABLE A-3-121

## CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROBENZENE (118-74-1)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.53E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	7.993E-03
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	9.68E-03
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.53E+00
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	6.31E-03
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—see Appendix A-3.	B-4-27	5.52E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	8.0E-04
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	1.6E+00
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	2.8E-03
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S. EPA (1997b)	C-2-1	4.6E-04
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	1.6E+00

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



**TABLE A-3-121**

**CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROBENZENE (118-74-1)**

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TABLE A-3-122

## CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROCYCLOPENTADIENE (77-47-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Montgomery and Welkom (1991)	--	272.77
$T_m$ (K)	Montgomery and Welkom (1991)	--	264.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	9.63E-05 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.53E+00
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.72E-02
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.61E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.21E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	8.07E_04
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	9.51E+03
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.51E+01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.13E+2

TABLE A-3-122

## CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROCYCLOPENTADIENE (77-47-4)

Parameter	Reference and Explanation	Equations	Value
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.80E+02
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.40E+03
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	1.47E+01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	5.65E-02
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	5.65E-02
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	5.47E-01

TABLE A-3-122

## CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROCYCLOPENTADIENE (77-47-4)

Parameter	Reference and Explanation	Equations	Value
$B_{V_{forage}}$ $\left(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}}\right)$	$B_{V_{forage}}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	5.47E-01
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	6.41E-04
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.03E-03
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	2.45E-03
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	6.41E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	1.60E-03
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	5.25E+02
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	7.00E-03
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997c)	C-2-3	7.00E-05
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

**TABLE A-3-122**

**CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROCYCLOPENTADIENE (77-47-4)**

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-123

## CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROETHANE (67-72-1)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, Heckelman (1989)	--	236.74
$T_m$ (K)	Montgomery and Welkom (1991)	--	459.7
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	6.21E-04 at 25°C (solid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	4.08E+01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.60E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.77E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.88E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	9.66E+03
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.82E+04
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.82E+01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.36E+01

TABLE A-3-123

## CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROETHANE (67-72-1)

Parameter	Reference and Explanation	Equations	Value
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	7.27E+01
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.78E+02
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	1.53E+01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{leafyveg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.93E-01
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.93E-01
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{leafyveg}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990; 1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-9	2.72E-01

TABLE A-3-123

## CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROETHANE (67-72-1)

Parameter	Reference and Explanation	Equations	Value
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1990; 1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-9	2.72E-01
<b>Biotransfer Factors for Animals (Continued)</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	7.67E-05
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.43E-04
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.2 of Appendix A-3).	B-3-12	2.94E-04
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	7.67E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.3 of Appendix A-3).	B-3-14	1.92E-04
$BCF_{fish}$ (L/kg, FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF$ values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—See Appendix A-3.	B-4-26	6.29E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.00E-03
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	1.40E-02
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	3.50E-03
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S. EPA (1997b)	C-2-1	4.00E-06
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	1.40E-02

Note:

NA = Not applicable



**TABLE A-3-123**

**CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROETHANE (67-72-1)**

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-124

## CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROPHENE (70-30-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith and Heckleman (1989)	--	406.92
$T_m$ (K)	Budavari, O'Neil, Smith and Heckleman (1989)	--	437.1
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b).	--	3.60E-15 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	3.0E-03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.88E-10
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.46E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.01E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	3.47E+ 07
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.08E+ 06
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.08E+ 04
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.08E+ 04
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	4.31E+ 04

TABLE A-3-124

## CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROPHENE (70-30-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.71E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.4E-04
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.49E+05
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	1.38E+00
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.70E-03
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.70E-03
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.23E+10
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.23E+10

TABLE A-3-124

## CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROPHENE (70-30-4)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.75E-01
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	8.71E-01
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.2 of Appendix A-3).	B-3-12	1.05E+00
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.75E+02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.2 of Appendix A-3).	B-3-14	6.88E-01
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	4.66E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.00E-04
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.10E-03
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-125

## CHEMICAL-SPECIFIC INPUTS FOR HYDROGEN CHLORIDE (7647-01-0)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	36.47
$T_m$ (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	158.9
$V_p$ (atm)	U.S. EPA (1994b)	--	4.6E+01 (liquid)
$S$ (mg/L)	--	--	ND
$H$ (atm·m <sup>3</sup> /mol)	--	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	ND
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.73E-01
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	2.00E-05
$K_{ow}$ (unitless)	--	--	NA
$K_{oc}$ (mL/g)	--	--	NA
$Kd_s$ (mL/g)	--	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	ND
$Kd_{sw}$ (L/Kg)	--	B-4-16; B-4-18; B-4-24	ND
$Kd_{bs}$ (mL/g)	--	B-4-16; B-4-25	ND
$k_{sg}$ (year) <sup>-1</sup>	--	B-1-2; B-2-2; B-3-2; B-4-2	ND
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0

TABLE A-3-125

## CHEMICAL-SPECIFIC INPUTS FOR HYDROGEN CHLORIDE (7647-01-0)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g WW plant}}{\mu\text{g/mL soil water}})$	--	B-2-10	ND
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	--	B-2-10	ND
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	--	B-2-9	ND
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	--	B-3-9	ND
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	--	B-2-8	NA
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	--	B-3-8	NA
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	--	B-3-11	ND
$Ba_{beef}$ (day/kg FW)	--	B-3-10	ND
$Ba_{pork}$ (day/kg FW)	--	B-3-12	ND
$BCF_{egg}$ (day/kg FW)	--	B-3-13	ND
$BCF_{chick}$ (day/kg FW)	--	B-3-14	ND
$BCF_{fish}$ (L/kg FW)	--	B-4-26	ND
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA

TABLE A-3-125

## CHEMICAL-SPECIFIC INPUTS FOR HYDROGEN CHLORIDE (7647-01-0)

Parameter	Reference and Explanation	Equations	Value
<b>Health Benchmarks</b>			
<i>RfD</i> (mg/kg/day)	Calculated from <i>RfC</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-1-8	5.7E-03
<i>Oral CSF</i> (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
<i>RfC</i> (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	2.0E-02
<i>Inhalation URF</i> (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
<i>Inhalation CSF</i> (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-126

## CHEMICAL-SPECIFIC INPUTS FOR INDENO(1,2,3-CD)PYRENE (193-39-5)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Montgomery and Welkom (1991)	--	276.34
$T_m$ (K)	Montgomery and Welkom (1991)	--	435
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	1.88E-13 at 25°C (solid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	1.07E-02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.86E-09
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from WATER8 model database U.S. EPA (1995d)	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.90E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from WATER8 model database U.S. EPA (1995d)	B-4-20	5.66E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	8.22E+06
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	4.11E+06
$Kd_s$ (mL/g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.11E+04
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.08E+05
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.64E+05
<b>Chemical/Physical Properties (Continued)</b>			



TABLE A-3-126

## CHEMICAL-SPECIFIC INPUTS FOR INDENO(1,2,3-CD)PYRENE (193-39-5)

Parameter	Reference and Explanation	Equations	Value
$k_{sg} \text{ (year)}^{-1}$	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.47E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.007
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	4.91E+04
$Br_{root \text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	1.19E+00
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.90E-03
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.90E-03
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	2.67E+08
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	2.67E+08

TABLE A-3-126

## CHEMICAL-SPECIFIC INPUTS FOR INDENO(1,2,3-CD)PYRENE (193-39-5)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	6.53E-02
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.07E-01
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	2.50E-01
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	6.53E+01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.63E-01
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	1.31E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	Calculated by multiplying the $Oral\ CSF$ for Benzo(a)pyrene by the relative potency factor for Indeno(1,2,3-cd)pyrene of 0.1 (U.S.EPA 1993e).	C-1-7	7.3E-01
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	2.1E-04
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	7.3E-01

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-127

## CHEMICAL-SPECIFIC INPUTS FOR ISOPHORONE (78-59-1)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Montgomery and Welkom (1991)	--	138.21
$T_m$ (K)	Montgomery and Welkom (1991)	--	265.1
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1992a).	--	7.08E-07 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.20E+04
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	8.15E-09
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.22E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.50E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	5.00E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	2.99E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.99E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.25E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.20E+00

TABLE A-3-127

## CHEMICAL-SPECIFIC INPUTS FOR ISOPHORONE (78-59-1)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.10E+01
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	3.68E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	4.04E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	4.04E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	4.42E+02
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	4.42E+02

TABLE A-3-127

## CHEMICAL-SPECIFIC INPUTS FOR ISOPHORONE (78-59-1)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	3.97E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.26E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.52E-06
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	3.97E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	9.92E-07
$BCF_{fish}$ (L/kg, FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.15E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.00E-01
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S.EPA (1997b)	C-1-7	9.50E-04
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	7.00E-01
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	2.70E-07
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	9.50E-04

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-128

## CHEMICAL-SPECIFIC INPUTS FOR LEAD (7439-92-1)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	207.2
$T_m$ (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	600.5
$V_p$ (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
$S$ (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	--	0.0
$H$ (atm·m <sup>3</sup> /mol)	$H$ value is assumed to be zero, because the $V_p$ and $S$ values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.43E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	6.28E-06
$K_{ow}$ (unitless)	--	--	NA
$K_{oc}$ (mL/g)	--	--	NA
$Kd_s$ (mL/g)	$Kd_s$ value was obtained from Baes, Sharp, Sjoreen, and Shor (1984), which states that several factors, such as experimental methods and soil type, could influence partitioning or $Kd_s$ values. Baes, Sharp, Sjoreen, and Shor (1984) compares values between various literature sources and provide this value, which is based on its best judgment.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.00E+02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value is assumed to be same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	9.00E+02
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value is assumed to be same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	9.00E+02
$k_{sg}$ (year) <sup>-1</sup>	--	B-1-2; B-2-2; B-3-2; B-4-2	ND

TABLE A-3-128

## CHEMICAL-SPECIFIC INPUTS FOR LEAD (7439-92-1)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
<i>Fv</i> (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.0
<b>Biotransfer Factors for Plants</b>			
<i>RCF</i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	--	B-2-10	ND
<i>Br<sub>root veg</sub></i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	<i>Br<sub>root veg</sub></i> value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). <i>Br</i> values for nonvegetative growth (such as tubers) in Baes, Sharp, Sjoreen, and Shor (1984) were used for <i>Br<sub>root veg</sub></i> .	B-2-10	9.00E-03
<i>Br<sub>ag</sub></i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	<i>Br<sub>ag</sub></i> value for fruits was obtained from Baes, Sharp, Sjoreen, and Shor (1984). <i>Br</i> values for nonvegetative growth (reproductive) in Baes, Sharp, Sjoreen, and Shor (1984) were used for <i>Br<sub>ag</sub></i> (fruits). <i>Br<sub>ag</sub></i> value for vegetables was calculated using data obtained from Baes, Sharp, Sjoreen, and Shor (1984). <i>Br</i> values for nonvegetative (reproductive) growth and <i>Bv</i> values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjoreen, and Shor [1984])—were used for <i>Br<sub>ag</sub></i> (vegetables). The weighted average <i>Br<sub>ag</sub></i> value for aboveground produce was obtained as follows: (1) <i>Br<sub>ag</sub></i> values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) <i>Br<sub>ag</sub></i> values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	1.36E-02
<i>Br<sub>forage</sub></i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	<i>Br<sub>forage</sub></i> value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). <i>Bv</i> values for vegetative growth (such as leaves and stems) in Baes, Sharp, Sjoreen, and Shor (1984) were used for <i>Br<sub>forage</sub></i> .	B-3-8	4.50E-02
<i>Br<sub>grain</sub></i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	<i>Br<sub>grain</sub></i> value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). <i>Br</i> values for nonvegetative growth as recommended by Baes, Sharp, Sjoreen, and Shor (1984) were used for <i>Br<sub>grain</sub></i> .	B-3-8	9.00E-03
<i>Bv<sub>ag</sub></i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA

TABLE A-3-128

## CHEMICAL-SPECIFIC INPUTS FOR LEAD (7439-92-1)

Parameter	Reference and Explanation	Equations	Value
$Bv_{forage}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ air}})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-11	2.5E-04
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-10	3.0E-04
$Ba_{pork}$ (day/kg FW)	NC DEHNR (1997)	B-3-12	3.6E-04
$Ba_{egg}$ (L/kg FW)	--	B-3-13	ND
$Ba_{chicken}$ (day/kg FW)	--	B-3-14	ND
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	ND
$BAF_{fish}$ (day/kg FW)	Because lead is hydrophobic, $BAF$ was used. $BAF_{fish}$ value was obtained from NC DEHNR (1997).	B-4-27	8.0
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	--	C-1-8	ND
$Oral \text{ CSF}$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	ND
$Inhalation \text{ URF}$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation \text{ CSF}$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-129

## CHEMICAL-SPECIFIC INPUTS FOR MALATHIONE (121-75-5)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	330.36
$T_m$ (K)	Montgomery and Welkom (1991)	--	276
$V_p$ (atm)	$V_p$ value cited in Howard (1989-1993).	--	1.04E-08 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in Howard (1989-1993).	--	1.43E+02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.40E-08
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.47E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.29E-06
$K_{ow}$ (unitless)	Recommended $K_{ow}$ value cited in Karickhoff and Long (1995).	--	2.29E+02
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	9.81E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.81E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.36E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.92E+00

TABLE A-3-129

## CHEMICAL-SPECIFIC INPUTS FOR MALATHIONE (121-75-5)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.946
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.16E+01
$Br_{root \text{ veg}}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	2.20E+01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.68E+00
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.68E+00
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	7.58E+02
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	7.58E+02

TABLE A-3-129

## CHEMICAL-SPECIFIC INPUTS FOR MALATHIONE (121-75-5)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.82E-06
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	5.75E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	6.96E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.82E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	4.54E-06
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	3.66E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.0E-02
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	7.0E-02
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-130

## CHEMICAL-SPECIFIC INPUTS FOR MERCURIC CHLORIDE (7487-94-7)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	271.52
$T_m$ (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	550.1
$V_p$ (atm)	U.S. EPA (1996a)	--	1.20E-04
$S$ (mg/L)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	6.90E+04
$H$ (atm·m <sup>3</sup> /mol)	U.S. EPA (1997g)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.1E-10
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1997g).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.53E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	5.25E-06
$K_{ow}$ (unitless)	U.S. EPA (1996a)	--	6.10E-01
$K_{oc}$ (mL/g)	--	--	NA
$Kd_s$ (mL/g)	U.S. EPA (1997g)	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.80E+04
$Kd_{sw}$ (L/Kg)	U.S. EPA (1997g)	B-4-16; B-4-18; B-4-24	1.00E+05
$Kd_{ps}$ (mL/g)	U.S. EPA (1997g)	B-4-16; B-4-25	5.00E+04
$ksg$ (year) <sup>-1</sup>	U.S. EPA (1996a)	B-1-2; B-2-2; B-3-2; B-4-2	0.0
$Fv$ (unitless)	Estimated based on discussions concerning divalent mercury provided in U.S. EPA (1996a).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.85

TABLE A-3-130

## CHEMICAL-SPECIFIC INPUTS FOR MERCURIC CHLORIDE (7487-94-7)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g WW plant}}{\mu\text{g/mL soil water}})$	--	B-2-10	ND
$Br_{\text{rootveg}}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	U.S. EPA (1997g)	B-2-10	3.60E-02
$Br_{\text{ag}}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{\text{ag}}$ value for fruits was obtained from Baes, Sharp, Sjoeren, and Shor (1984). $Br$ values for nonvegetative growth (reproductive) in Baes, Sharp, Sjoeren, and Shor (1984) were used for $Br_{\text{ag}}$ (fruits). $Br_{\text{ag}}$ value for vegetables was calculated using data obtained from Baes, Sharp, Sjoeren, and Shor (1984). $Br$ values for nonvegetative (reproductive) growth and $Bv$ values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjoeren, and Shor [1984])—were used for $Br_{\text{ag}}$ (vegetables). The weighted average $Br_{\text{ag}}$ value for aboveground produce was obtained as follows: (1) $Br_{\text{ag}}$ values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) $Br_{\text{ag}}$ values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	1.45E-02
$Br_{\text{forage}}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	U.S. EPA (1997g)	B-3-9	0.0
$Bv_{\text{ag}}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	U.S. EPA (1997g)	B-2-8	1.8E+03
$Bv_{\text{forage}}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	U.S. EPA (1997g)	B-3-8	1.8E+03
<b>Biotransfer Factors for Animals</b>			
$Ba_{\text{milk}}$ (day/kg FW)	Default $Ba_{\text{milk}}$ (dry weight value) obtained from U.S. EPA (1997g) was converted to a wet weight basis assuming a 87% moisture content in milk. U.S. EPA U.S. EPA (1997g) does not differentiate between different forms of mercury. Mercury is assumed to be in the form of 87% divalent mercury and 13% methyl mercury in herbivore animals. Therefore, the calculated $Ba_{\text{milk}}$ (wet weight) value was multiplied by 0.87.	B-3-11	2.26E-03

TABLE A-3-130

## CHEMICAL-SPECIFIC INPUTS FOR MERCURIC CHLORIDE (7487-94-7)

Parameter	Reference and Explanation	Equations	Value
$Ba_{beef}$ (day/kg FW)	Default $Ba_{beef}$ (dry weight value) obtained from U.S. EPA (1997g) was converted to a wet weight basis assuming a 70% moisture content in beef. U.S. EPA (1997g) does not differentiate between different forms of mercury. Mercury is assumed to be in the form of 87% divalent mercury and 13% methyl mercury in herbivore animals. Therefore, the calculated $Ba_{beef}$ (wet weight) value was multiplied by 0.87.	B-3-10	5.22E-03
$Ba_{pork}$ (day/kg FW)	Default $Ba_{pork}$ (dry weight value) of 0.00013 day/kg DW obtained from U.S. EPA (1997g) was converted to a wet weight basis assuming a 70 % moisture content in pork. U.S. EPA (1997g) does not differentiate between different forms of mercury. Mercury is assumed to be in the form of 87% divalent mercury and 13% methyl mercury in herbivore animals. Therefore, the calculated $Ba_{pork}$ (wet weight) value was multiplied by 0.87.	B-3-12	3.39E-05
$Ba_{egg}$ (day/kg FW)	Default $Ba_{egg}$ (dry weight value) of 0.11 day/kg DW obtained from U.S. EPA (1997g) was converted to a wet weight basis assuming a 75 % moisture content in eggs. U.S. EPA (1997g) does not differentiate between different forms of mercury. Mercury is assumed to be in the form of 87% divalent mercury and 13% methyl mercury in herbivore animals. Therefore, the calculated $Ba_{egg}$ (wet weight) value was multiplied by 0.87.	B-3-13	2.39E-02
$Ba_{chicken}$ (day/kg FW)	Default $Ba_{chicken}$ (dry weight value) of 0.11 day/kg DW obtained from U.S. EPA (1997g) was converted to a wet weight basis assuming a 75 % moisture content in chicken. U.S. EPA (1997g) does not differentiate between different forms of mercury. Mercury is assumed to be in the form of 87% divalent mercury and 13% methyl mercury in herbivore animals. Therefore, the calculated $Ba_{chicken}$ (wet weight) value was multiplied by 0.87.	B-3-14	2.39E-02
$BCF_{fish}$ (L/kg FW)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1997b)	C-1-8	3.0E-04
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.1E-03

TABLE A-3-130

## CHEMICAL-SPECIFIC INPUTS FOR MERCURIC CHLORIDE (7487-94-7)

Parameter	Reference and Explanation	Equations	Value
<b>Health Benchmarks (Continued)</b>			
<i>Inhalation URF</i> ( $\mu\text{g}/\text{m}^3$ ) <sup>-1</sup>	--	C-2-1	ND
<i>Inhalation CSF</i> ( $\text{mg}/\text{kg}/\text{day}$ ) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not Applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-131

## CHEMICAL-SPECIFIC INPUTS FOR MERCURY (7439-97-6)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	200.59
$T_m$ (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	234.23
$V_p$ (atm)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	2.63E-06 at 25°C
$S$ (mg/L)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	5.62E-02
$H$ (atm·m <sup>3</sup> /mol)	U.S. EPA (1997g)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.1E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database in U.S. EPA (1994d). CHEMDAT8 uses correlations with density and molecular weight to calculate $D_a$ values. A density value of 13.546 g/cc for mercury was used.	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.09E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database in U.S. EPA (1994d). CHEMDAT8 uses correlations with density and molecular weight to calculate $D_w$ values. A density value of 13.546 g/cc for mercury was used.	B-4-20	3.01E-05
$K_{ow}$ (unitless)	--	--	NA
$K_{oc}$ (mL/g)	--	--	NA
$Kd_s$ (mL/g)	U.S.EPA (1997g)	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.00E+03
$Kd_{sw}$ (L/Kg)	U.S.EPA (1997g)	B-4-16; B-4-18; B-4-24	1.00E+03
$Kd_{bs}$ (mL/g)	U.S.EPA (1997g)	B-4-16; B-4-25	3.00E+03
$k_{sg}$ (yr) <sup>-1</sup>	U.S. EPA (1996a)	B-1-2; B-2-2; B-3-2; B-4-2	0.0



TABLE A-3-131

## CHEMICAL-SPECIFIC INPUTS FOR MERCURY (7439-97-6)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	--	B-2-10	ND
$Br_{root\ veg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	Elemental mercury does not deposit onto soils. Therefore, it is assumed that there is no plant uptake through the soil.	B-2-10	NA
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value for fruits was obtained from Baes, Sharp, Sjoreen, and Shor (1984). $Br$ values for nonvegetative growth (reproductive) in Baes, Sharp, Sjoreen, and Shor (1984) were used for $Br_{ag}$ (fruits). $Br_{ag}$ value for vegetables was calculated using data obtained from Baes, Sharp, Sjoreen, and Shor (1984). $Br$ values for nonvegetative (reproductive) growth and $B_v$ values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjoreen, and Shor [1984])—were used for $Br_{ag}$ (vegetables). The weighted average $Br_{ag}$ value for aboveground produce was obtained as follows: (1) $Br_{ag}$ values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) $Br_{ag}$ values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	NA
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	Elemental mercury is assumed not to deposit onto soils. Therefore, it is assumed that there is no transfer of mercury to the aboveground plant parts through root uptake.	B-3-8	NA
$Br_{grain}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	Elemental mercury is assumed not to deposit onto soils. Therefore, it is assumed that there is no transfer of mercury to the aboveground plant parts through root uptake.	B-3-8	NA
$B_{v_{ag}}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	Elemental mercury exists in very low concentrations in the vapor phase. Therefore, $B_{v_{ag}}$ value for elemental mercury is not modeled for the indirect exposure pathways. Elemental mercury is modeled for the inhalation pathway only. No literature data is available to calculate a $B_{v_{ag}}$ value for elemental mercury.	B-2-8	ND

TABLE A-3-131

## CHEMICAL-SPECIFIC INPUTS FOR MERCURY (7439-97-6)

Parameter	Reference and Explanation	Equations	Value
$Bv_{forage}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ air}})$	Elemental mercury exists in very low concentrations in the vapor phase. Therefore, $Bv_{forage}$ value for elemental mercury is not modeled for the indirect exposure pathways. Elemental mercury is modeled for the inhalation pathway only. No literature data is available to calculate a $Bv_{forage}$ value for elemental mercury.	B-3-8	ND
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	Elemental mercury does not deposit onto soils nor gets transferred to the aboveground plant parts. Therefore, there is no transfer of elemental mercury into the animal tissue.	B-3-11	NA
$Ba_{beef}$ (day/kg FW)	Elemental mercury does not deposit onto soils nor gets transferred to the aboveground plant parts. Therefore, there is no transfer of elemental mercury into the animal tissue.	B-3-10	NA
$Ba_{pork}$ (day/kg FW)	Elemental mercury does not deposit onto soils nor gets transferred to the aboveground plant parts. Therefore, there is no transfer of elemental mercury into the animal tissue.	B-3-12	NA
$Ba_{egg}$ (day/kg FW)	Elemental mercury does not deposit onto soils nor gets transferred to the aboveground plant parts. Therefore, there is no transfer of elemental mercury into the animal tissue.	B-3-13	NA
$Ba_{chicken}$ (day/kg FW)	Elemental mercury does not deposit onto soils nor gets transferred to the aboveground plant parts. Therefore, there is no transfer of elemental mercury into the animal tissue.	B-3-14	NA
$BCF_{fish}$ (L/g FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	Elemental mercury does not deposit onto soils and surface water. Therefore, there is no transfer of elemental mercury into the fish tissue.	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	Calculated from $RfC$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-1-8	8.60E-05
$Oral \text{ CSF}$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	3.0E-04
$Inhalation \text{ URF}$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation \text{ CSF}$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not available

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-132

## CHEMICAL-SPECIFIC INPUTS FOR METHACRYLONITRILE (126-98-7)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	67.09
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	237.3
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b)	--	8.90E-02 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b)	--	2.50E+04
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.39E-04
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.15E-01
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	1.33E-05
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	--	3.47E+00
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	3.74E+00
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.74E-02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.80E-01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.49E-01

TABLE A-3-132

## CHEMICAL-SPECIFIC INPUTS FOR METHACRYLONITRILE (126-98-7)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was assumed to be zero due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.91E+00
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	1.85E+02
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.89E+01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.89E+01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	8.81E-04
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	8.81E-04

TABLE A-3-132

## CHEMICAL-SPECIFIC INPUTS FOR METHACRYLONITRILE (126-98-7)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.76E-08
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	8.72E-08
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.06E-07
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.76E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	6.88E-08
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.52E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.0E-04
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997c)	C-2-3	7.0E-04
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-133

## CHEMICAL-SPECIFIC INPUTS FOR METHANOL (67-56-1)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	32.04
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	175.3
$V_p$ (atm)	$V_p$ value cited in Montgomery and Welkom (1991)	--	1.30E-01 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b)	--	2.90E+04
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.44E-04
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.58E-01
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.64E-05
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	--	1.95E-01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	3.96E-01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.96E-03
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.97E-02

TABLE A-3-133

## CHEMICAL-SPECIFIC INPUTS FOR METHANOL (67-56-1)

Parameter	Reference and Explanation	Equations	Value
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.58E-02
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.37E+00
$Br_{root\ veg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.61E+03
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	9.96E+01
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	9.96E+01
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	6.82E-05
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	6.82E-05

TABLE A-3-133

## CHEMICAL-SPECIFIC INPUTS FOR METHANOL (67-56-1)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.30E-09
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	4.30E-09
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	5.21E-09
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.55E-06
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	3.39E-09
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.70E-01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.00E-01
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.8E+00
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-134

## CHEMICAL-SPECIFIC INPUTS FOR METHOXYCHLOR (72-43-5)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	345.65
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	351.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.62E-09 at 25°C (solid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	8.84E-02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.33E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.30E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.59E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	3.36E+ 04
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	8.00E+ 04
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.00E+ 02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.00E+ 03
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.20E+ 03

TABLE A-3-134

## CHEMICAL-SPECIFIC INPUTS FOR METHOXYCHLOR (72-43-5)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	6.93E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.901
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-10	7.16E+02
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	8.95E-01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	9.38E-02
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	9.38E-02
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	5.83E+02
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	5.83E+02

TABLE A-3-134

## CHEMICAL-SPECIFIC INPUTS FOR METHOXYCHLOR (72-43-5)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.67E-04
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	8.43E-04
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.2 of Appendix A-3).	B-3-12	1.02E-03
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.67E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.3 of Appendix A-3).	B-3-14	6.66E-04
$BCF_{fish}$ (L/kg, FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Carroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	3.16E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.00E-03
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.80E-02
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-135

## CHEMICAL-SPECIFIC INPUTS FOR METHYL ACETATE (79-20-9)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Montgomery and Welkom (1991)	--	74.08
$T_m$ (K)	Montgomery and Welkom (1991)	--	175.1
$V_p$ (atm)	$V_p$ value cited in Howard (1989-1993).	--	2.84E-01 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in Howard (1989-1993).	--	2.44E+05
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	8.64E-05
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.23E-01
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.10E-05
$K_{ow}$ (unitless)	Recommended $K_{ow}$ value cited in Karickhoff and Long (1995).	--	2.90E+00
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	3.25E+00
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.25E-02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.44E-01

TABLE A-3-135

## CHEMICAL-SPECIFIC INPUTS FOR METHYL ACETATE (79-20-9)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.30E-01
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.84E+00
$Br_{root\ veg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.10E+02
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.09E+01
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.09E+01
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	2.01E-03

TABLE A-3-135

## CHEMICAL-SPECIFIC INPUTS FOR METHYL ACETATE (79-20-9)

Parameter	Reference and Explanation	Equations	Value
$Bv_{forage}$ $\left(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}}\right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	2.01E-03
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.30E-08
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	7.28E-08
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	8.82E-08
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.30E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	5.75E-08
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.32E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997c)	C-1-8	1.00E+00
$Oral CSF$ (mg/kg/day) <sup>-1</sup>		C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	3.50E+01
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>		C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>		C-2-2	ND

Note:

NA = Not applicable

ND = No data available

## **TABLE A-3-135**

### **CHEMICAL-SPECIFIC INPUTS FOR METHYL ACETATE (79-20-9)**

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-136

## CHEMICAL-SPECIFIC INPUTS FOR METHYL BROMIDE (74-83-9)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith and Heckelman (1989)	--	94.95
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	179.44
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.16E+ 00 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.45E+ 04
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.41E-02
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.28E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.21E-05
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.30E+ 01
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	9.00E+ 00
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.00E-02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.75E-01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.60E-01



TABLE A-3-136

## CHEMICAL-SPECIFIC INPUTS FOR METHYL BROMIDE (74-83-9)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+ 00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	7.98E+00
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	8.87E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	8.79E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	8.79E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	6.07E-05
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	6.07E-05

TABLE A-3-136

## CHEMICAL-SPECIFIC INPUTS FOR METHYL BROMIDE (74-83-9)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.03E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.27E-07
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.2 of Appendix A-3).	B-3-12	3.95E-07
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.03E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.3 of Appendix A-3).	B-3-14	2.58E-07
$BCF_{fish}$ (L/kg, FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	4.14E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.40E-03
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	5.00E-03
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-137

## CHEMICAL-SPECIFIC INPUTS FOR METHYL CHLORIDE (74-87-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	50.49
$T_m$ (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	176.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	5.68E+ 00 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	6.34E+ 03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.52E-02
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.13E-01
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.39E-05
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	8.00E+ 00
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	6.00E+ 00
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	6.00E-02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	4.50E-01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.40E-01

TABLE A-3-137

## CHEMICAL-SPECIFIC INPUTS FOR METHYL CHLORIDE (74-87-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boehling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+ 00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	7.46E+00
$Br_{root \text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	1.24E+02
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.16E+01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.16E+01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.13E-05
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.13E-05

TABLE A-3-137

## CHEMICAL-SPECIFIC INPUTS FOR METHYL CHLORIDE (74-87-3)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	6.36E-08
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.01E-07
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.2 of Appendix A-3).	B-3-12	2.43E-07
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	6.35E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.3 of Appendix A-3).	B-3-14	1.59E-07
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	2.86E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	Calculated from $RfC$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-1-8	8.60E-02
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1995c)	C-1-7	1.30E-02
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997d)	C-2-3	3.00E-01
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S. EPA (1995b)	C-2-1	1.80E-06
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1995b)	C-2-2	6.30E-03

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-138

## CHEMICAL-SPECIFIC INPUTS FOR METHYL ETHYL KETONE (78-93-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	72.10
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	187.1
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b).	--	1.20E-01 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	2.40E+05
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.61E-05
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.35E-01
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.03E-05
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	1.91E+00
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	2.34E+00
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.34E-02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.76E-01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	9.36E-02

TABLE A-3-138

## CHEMICAL-SPECIFIC INPUTS FOR METHYL ETHYL KETONE (78-93-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.69E+00
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.86E+02
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.67E+01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.67E+01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	3.08E-03
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	3.08E-03

TABLE A-3-138

## CHEMICAL-SPECIFIC INPUTS FOR METHYL ETHYL KETONE (78-93-3)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.51E-08
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	4.79E-08
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	5.79E-08
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.51E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	3.78E-08
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	9.61E-01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	6.00E-01
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	1.00E+00
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-139

## CHEMICAL-SPECIFIC INPUTS FOR METHYL ISOBUTYL KETONE (108-10-1)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	100.16
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	188.4
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b).	--	2.50E-02 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	2.00E+04
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.25E-04
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	8.59E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.36E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	1.55E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.20E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.20E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	9.00E-01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	4.80E-01

TABLE A-3-139

## CHEMICAL-SPECIFIC INPUTS FOR METHYL ISOBUTYL KETONE (108-10-1)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.22E+00
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	6.85E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	7.95E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	7.95E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	8.26E-03
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	8.26E-03

TABLE A-3-139

## CHEMICAL-SPECIFIC INPUTS FOR METHYL ISOBUTYL KETONE (108-10-1)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.23E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.89E-07
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	4.71E-07
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.23E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	3.07E-07
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—see Appendix A-3.	B-4-26	4.73E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997c)	C-1-8	8.0E-02
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997a)	C-1-7	8.0E-01
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1995b)	C-2-3	8.0E-02
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from $Oral CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	2.3E-01
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	Value based on $Oral CSF$ assuming route-to-route extrapolation.	C-2-2	8.0E-01

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-140

## CHEMICAL-SPECIFIC INPUTS FOR METHYL MERCURY (22967-92-6)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	U.S. EPA (1997g)	--	216.0
$T_m$ (°K)	--	--	ND
$Vp$ (atm)	--	--	ND
$S$ (mg/L)	--	--	ND
$H$ (atm·m <sup>3</sup> /mol)	U.S. EPA (1997g)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.7E-07
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1997g).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.28E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	6.11E-06
$K_{ow}$ (unitless)	--	--	ND
$K_{oc}$ (mL/g)	--	--	ND
$Kd_s$ (mL/g)	USEPA (1997g)	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.00E+03
$Kd_{sw}$ (L/Kg)	USEPA (1997g)	B-4-16; B-4-18; B-4-24	1.00E+05
$Kd_{bs}$ (mL/g)	USEPA (1997g)	B-4-16; B-4-25	3.00E+03
$ksg$ (year) <sup>-1</sup>	U.S. EPA (1996a)	B-1-2; B-2-2; B-3-2; B-4-2	0.0
$Fv$ (unitless)	Based on discussions provided in U.S. EPA (1996a), methyl mercury does not exist in the air/vapor phase.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.0

TABLE A-3-140

## CHEMICAL-SPECIFIC INPUTS FOR METHYL MERCURY (22967-92-6)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	--	B-2-10	ND
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	U.S. EPA (1997g)	B-2-10	9.9E-02
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value for fruits was obtained from Baes, Sharp, Sjoeren, and Shor (1984). $Br$ values for nonvegetative growth (reproductive) in Baes, Sharp, Sjoeren, and Shor (1984) were used for $Br_{ag}$ (fruits). $Br_{ag}$ value for vegetables was calculated using data obtained from Baes, Sharp, Sjoeren, and Shor (1984). $Br$ values for nonvegetative (reproductive) growth and $Bv$ values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjoeren, and Shor [1984])—were used for $Br_{ag}$ (vegetables). The weighted average $Br_{ag}$ value for aboveground produce was obtained as follows: (1) $Br_{ag}$ values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) $Br_{ag}$ values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	2.94E-02
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	U.S. EPA (1997g)	B-3-9	0.0
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	Methyl mercury is assumed not to exist in the air phase. Therefore, there is no biotransfer of methyl mercury from air into plants.	B-2-8	NA
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	Methyl mercury is assumed not to exist in the air phase. Therefore, there is no biotransfer of methyl mercury from air into plants.	B-3-8	NA
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	Default $Ba_{milk}$ (dry weight value) of 0.02 day/kg DW for mercury obtained from U.S. EPA (1997g) was converted to a wet weight basis assuming a 87% moisture content in milk. U.S. EPA (1997g) does not differentiate between different forms of mercury. Mercury is assumed to be in the form of 87% divalent mercury and 13% methyl mercury in herbivore animals. Therefore, the calculated $Ba_{milk}$ (wet weight) value was multiplied by 0.13.	B-3-11	3.38E-04

TABLE A-3-140

## CHEMICAL-SPECIFIC INPUTS FOR METHYL MERCURY (22967-92-6)

Parameter	Reference and Explanation	Equations	Value
$Ba_{beef}$ (day/kg FW)	Default $Ba_{beef}$ (dry weight value) of 0.02 day/kg DW obtained from U.S. EPA (1997g) was converted to a wet weight basis assuming a 70% moisture content in beef. U.S. EPA (1997g) does not differentiate between different forms of mercury. Mercury is assumed to be in the form of 87% divalent mercury and 13% methyl mercury in herbivore animals. Therefore, the calculated $Ba_{beef}$ (wet weight) value was multiplied by 0.13.	B-3-10	7.80E-04
$Ba_{pork}$ (day/kg FW)	Default $Ba_{pork}$ (dry weight value) of 0.00013 day/kg DW obtained from U.S. EPA (1997g) was converted to a wet weight basis assuming a 70 % moisture content in pork. U.S. EPA (1997g) does not differentiate between different forms of mercury. Mercury is assumed to be in the form of 87% divalent mercury and 13% methyl mercury in herbivore animals. Therefore, the calculated $Ba_{pork}$ (wet weight) value was multiplied by 0.13.	B-3-12	5.07E-06
$Ba_{egg}$ (day/kg FW)	Default $Ba_{egg}$ (dry weight value) of 0.11 day/kg DW obtained from U.S. EPA (1997g) was converted to a wet weight basis assuming a 75 % moisture content in eggs. U.S. EPA (1997g) does not differentiate between different forms of mercury. Mercury is assumed to be in the form of 87% divalent mercury and 13% methyl mercury in herbivore animals. Therefore, the calculated $Ba_{egg}$ (wet weight) value was multiplied by 0.13.	B-3-13	3.58E-03
$Ba_{chicken}$ (day/kg FW)	Default $Ba_{chicken}$ (dry weight value) of 0.11 day/kg DW obtained from U.S. EPA (1997g) was converted to a wet weight basis assuming a 75 % moisture content in chicken. U.S. EPA (1997g) does not differentiate between different forms of mercury. Mercury is assumed to be in the form of 87% divalent mercury and 13% methyl mercury in herbivore animals. Therefore, the calculated $Ba_{chicken}$ (wet weight) value was multiplied by 0.13.	B-3-14	3.58E-03
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	Default value cited in U.S. EPA (1997g) for a Trophic Level 4 fish.	B-4-27	6.80E+06
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.0E-04
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $Oral CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	3.5E-04
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not Applicable

ND = No data available

**TABLE A-3-140**

**CHEMICAL-SPECIFIC INPUTS FOR METHYL MERCURY (22967-92-6)**

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-141

## CHEMICAL-SPECIFIC INPUTS FOR METHYL PARATHION (298-00-0)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	263.23
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	310.1
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1992a).	--	1.30E-08 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1992a).	--	5.00E+01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.84E-08
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.87E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	6.43E-06
$K_{ow}$ (unitless)	$K_{ow}$ value cited in U.S. EPA (1995b).	--	7.20E+02
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	2.40E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.40E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.80E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	9.59E+00



TABLE A-3-141

## CHEMICAL-SPECIFIC INPUTS FOR METHYL PARATHION (298-00-0)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.03E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.966
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	4.31E+01
$Br_{root \text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.80E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	8.64E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	8.64E-01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	9.02E+02
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	9.02E+02

TABLE A-3-141

## CHEMICAL-SPECIFIC INPUTS FOR METHYL PARATHION (298-00-0)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	5.72E-06
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.81E-05
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	2.19E-05
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	5.72E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.43E-05
$BCF_{fish}$ (L/kg, FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	8.74E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.54E-04
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	8.8E-04
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-142

## CHEMICAL-SPECIFIC INPUTS FOR METHYLENE BROMIDE (74-95-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	173.86
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	220.4
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b).	--	2.20E+ 00 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	1.45E+ 04
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.64E-02
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.10E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	7.06E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	4.17E+ 01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	2.60E-01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.60E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.95E+ 00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.04E+ 00

TABLE A-3-142

## CHEMICAL-SPECIFIC INPUTS FOR METHYLENE BROMIDE (74-95-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.04E+01
$Br_{root \text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	4.01E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	4.48E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	4.48E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.13E-04
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.13E-04

TABLE A-3-142

## CHEMICAL-SPECIFIC INPUTS FOR METHYLENE BROMIDE (74-95-3)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	3.31E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.05E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.2 of Appendix A-3).	B-3-12	1.27E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	3.31E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.3 of Appendix A-3).	B-3-14	8.27E-07
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.00E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997c)	C-1-8	1.0E-02
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	3.5E-02
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-143

## CHEMICAL-SPECIFIC INPUTS FOR METHYLENE CHLORIDE (75-09-2)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	84.94
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	178.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	4.87E-01 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.74E+04
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.38E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	8.69E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.25E-05
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.80E+01
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.00E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.00E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.50E-01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	4.00E-01

TABLE A-3-143

## CHEMICAL-SPECIFIC INPUTS FOR METHYLENE CHLORIDE (75-09-2)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.46E+00
$Br_{root \text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	8.46E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	7.29E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	7.29E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	5.11E-04
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	5.11E-04

TABLE A-3-143

## CHEMICAL-SPECIFIC INPUTS FOR METHYLENE CHLORIDE (75-09-2)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.43E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	4.52E-07
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	5.47E-07
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.43E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	3.57E-07
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	5.30E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	6.0E-02
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	7.5E-03
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997c)	C-2-3	3.0E+00
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S. EPA (1997b)	C-2-1	4.7E-07
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	Calculated from the Inhalation URF using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-2	1.6E-03

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-144

## CHEMICAL-SPECIFIC INPUTS FOR NAPHTHALENE (91-20-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	128.16
$T_m$ (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	353.3
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.17E-04 at 25°C (solid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	3.11E+01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.82E-04
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.26E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-4-20	8.92E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	2.36E+03
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.19E+03
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.19E+01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.93E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	4.76E+01

TABLE A-3-144

## CHEMICAL-SPECIFIC INPUTS FOR NAPHTHALENE (91-20-3)

Parameter	Reference and Explanation	Equations	Value
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	5.27E+00
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/mL \text{ soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	9.81E+01
$Br_{root \text{ veg}}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	8.23E+00
$Br_{ag}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	4.35E-01
$Br_{forage}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	4.35E-01
$Bv_{ag}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	4.52E-01
$Bv_{forage}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ air}})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	4.52E-01

TABLE A-3-144

## CHEMICAL-SPECIFIC INPUTS FOR NAPHTHALENE (91-20-3)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.87E-05
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	5.92E-05
<b>Biotransfer Factors for Animals (Continued)</b>			
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	7.16E-05
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.87E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	4.67E-05
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	2.15E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1995b)	C-1-8	4.0E-02
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.40E-01
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-145

## CHEMICAL-SPECIFIC INPUTS FOR NICKEL (7440-02-0)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	58.69
$T_m$ (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	1,828
$V_p$ (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
$S$ (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	--	0.0
$H$ (atm·m <sup>3</sup> /mol)	$H$ value is assumed to be zero, because the $V_p$ and $S$ values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.26E-01
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	1.46E-05
$K_{ow}$ (unitless)	--	--	NA
$K_{oc}$ (mL/g)	--	--	NA
$Kd_s$ (mL/g)	$Kd_s$ value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	16 at pH=4.9; 65 at pH=6.8; 1,900 at pH=8.0;
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value is assumed to be same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	16 at pH=4.9; 65 at pH=6.8; 1,900 at pH=8.0;
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value is assumed to be same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	16 at pH=4.9; 65 at pH=6.8; 1,900 at pH=8.0;
$k_{sg}$ (year) <sup>-1</sup>	--	B-1-2; B-2-2; B-3-2; B-4-2	ND

TABLE A-3-145

## CHEMICAL-SPECIFIC INPUTS FOR NICKEL (7440-02-0)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$F_v$ (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	--	B-2-10	ND
$Br_{\text{rootveg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{\text{rootveg}}$ value was calculated by multiplying the uptake slope factor with a conversion factor of $2 \times 10^9$ g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for root vegetables.	B-2-10	8.00E-03
$Br_{\text{ag}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{\text{ag}}$ value for fruits was calculated by multiplying the uptake slope factor with a conversion factor of $2 \times 10^9$ g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1993e) for garden fruits. $Br_{\text{ag}}$ value for vegetables was calculated by weighting the uptake slope factors for garden fruits (75%) and leafy vegetables (25%) and multiplying the result with a conversion factor of $2 \times 10^9$ g/ha soil. The uptake slope factors and the conversion factor were obtained from U.S. EPA (1993e). The weighted average $Br_{\text{ag}}$ value for aboveground produce was obtained as follows: (1) $Br_{\text{ag}}$ values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) $Br_{\text{ag}}$ values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	9.31E-03
$Br_{\text{forage}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{\text{forage}}$ value was calculated by multiplying the uptake slope factor with a conversion factor of $2 \times 10^9$ g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for leafy vegetables.	B-3-8	3.20E-02
$Br_{\text{grain}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{\text{grain}}$ value was calculated by multiplying the uptake slope factors with a conversion factor of $2 \times 10^9$ g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for grains/cereals.	B-3-8	6.00E-03
$Bv_{\text{ag}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA
$Bv_{\text{forage}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA

TABLE A-3-145

## CHEMICAL-SPECIFIC INPUTS FOR NICKEL (7440-02-0)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-11	1.0E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-10	6.0E-03
$Ba_{pork}$ (day/kg FW)	--	B-3-12	ND
$Ba_{egg}$ (day/kg FW)	--	B-3-13	NA
$Ba_{chicken}$ (day/kg FW)	--	B-3-14	NA
$BCF_{fish}$ (L/kg FW tissue)	Geometric mean value obtained from various literature sources (see Appendix A3.4).	B-3-26	3.07E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, FW tissue)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.0E-02
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	7.02E-02
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-146

## CHEMICAL-SPECIFIC INPUTS FOR 2-NITROANILINE (88-74-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	138.12
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	342.1
$V_p$ (atm)	$V_p$ value cited in Montgomery and Welcom (1991).	--	1.07E-05 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in Montgomery and Welcom (1991).	--	1.26E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.17E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.29E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.81E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	7.08E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	3.93E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.93E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.95E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.57E+01

TABLE A-3-146

## CHEMICAL-SPECIFIC INPUTS FOR 2-NITROANILINE (88-74-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was assumed to be 0 due to a lack of data.	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	0.0
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	1.25E+01
$Br_{root \text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	3.18E+00
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.30E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.30E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	4.47E+00
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	4.47E+00



TABLE A-3-146

## CHEMICAL-SPECIFIC INPUTS FOR 2-NITROANILINE (88-74-4)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	5.62E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.78E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	2.15E-06
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	5.62E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.40E-06
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.50E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997a)	C-1-8	6.00E-05
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	NA
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997c)	C-2-3	2.00E-04
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	NA
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	NA

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-147

## CHEMICAL-SPECIFIC INPUTS FOR 3-NITROANILINE (99-09-2)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	138.12
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	387.1
$V_p$ (atm)	--	--	1.07E-05 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in Montgomery and Welcom (1991)	--	8.90E+02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.65E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.11E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	8.23E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	2.34E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.66E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.66E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.24E+01

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## CHEMICAL-SPECIFIC INPUTS FOR 3-NITROANILINE (99-09-2)

Parameter	Reference and Explanation	Equations	Value
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	6.62E+00
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was assumed to be 0 due to a lack of data.	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	0.0
$F_v$ (unitless)	$F_v$ value was assumed to be 1.0 due to a lack of data.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/mL \text{ soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	8.94E+00
$Br_{rootveg}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	5.40E+00
$Br_{ag}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	6.26E+00
$Br_{forage}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	6.26E+00
$Bv_{ag}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	9.71E-01

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## CHEMICAL-SPECIFIC INPUTS FOR 3-NITROANILINE (99-09-2)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (Continued)</b>			
$Bv_{forage}$ $\left(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}}\right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	9.71E-01
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.86E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	5.88E-07
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	7.12E-07
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.86E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	4.64E-07
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF$ values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—see Appendix A-3.	B-4-26	5.92E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997a)	C-1-8	3.00E-03
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	NA
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.05E-02
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	NA
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	NA

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## CHEMICAL-SPECIFIC INPUTS FOR 4-NITROANILINE (100-01-6)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	138.12
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	419.10
$V_p$ (atm)	--	--	ND
$S$ (mg/L)	$S$ value cited in Montgomery and Welcom (1991)	--	1.07E-05
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.65E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.31E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.75E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	2.46E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.72E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.72E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.29E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	6.89E+00

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## CHEMICAL-SPECIFIC INPUTS FOR 4-NITROANILINE (100-01-6)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was assumed to be 0 due to a lack of data.	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	0.0
$F_v$ (unitless)	$F_v$ value was assumed to be 1.0 due to a lack of data.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	9.04E+00
$Br_{root \text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	5.25E+00
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	6.08E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	6.08E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.02E+00
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.02E+00

TABLE A-3-148

## CHEMICAL-SPECIFIC INPUTS FOR 4-NITROANILINE (100-01-6)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.95E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	6.18E-07
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	7.48E-07
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.95E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	4.88E-07
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	5.00E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997a)	C-1-8	3.00E-03
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	NA
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.05E-02
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	NA
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	NA

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-149

## CHEMICAL-SPECIFIC INPUTS FOR NITROBENZENE (98-95-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	123.11
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	279.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	3.21E-04 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	1.92E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.06E-05
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.43E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-4-20	9.43E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	6.80E+01
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.19E+02
$Kd_s$ (mL/g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.19E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.93E+00
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	4.76E+004



TABLE A-3-149

## CHEMICAL-SPECIFIC INPUTS FOR NITROBENZENE (98-95-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.28E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the liquid-phase $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.23E+01
$Br_{root\ veg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	1.03E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.38E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.38E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	2.43E-01
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	2.43E-01

TABLE A-3-149

## CHEMICAL-SPECIFIC INPUTS FOR NITROBENZENE (98-95-3)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	5.40E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.71E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	2.07E-06
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	5.40E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.35E-06
$BCF_{fish}$ (L/kg, FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF$ values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—See Appendix A-3.	B-4-26	5.92E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.0E-04
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	2.0E-03
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-150

## CHEMICAL-SPECIFIC INPUTS FOR 2-NITROPHENOL (88-75-5)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	139.11
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	317.1
$V_p$ (atm)	$V_p$ value cited in Howard (1989-1993).	--	2.63E-04 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in Howard (1989-1993).	--	2.50E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.46E-05
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.44E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.19E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	6.17E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	3.53E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.53E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.65E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.41E+01

TABLE A-3-150

## CHEMICAL-SPECIFIC INPUTS FOR 2-NITROPHENOL (88-75-5)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	9.03E+00
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	1.19E+01
$Br_{root \text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	3.36E+00
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.57E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.57E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	3.08E-01
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	3.08E-01

TABLE A-3-150

## CHEMICAL-SPECIFIC INPUTS FOR 2-NITROPHENOL (88-75-5)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	4.90E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.55E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.88E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	4.90E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.22E-06
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.35E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.